

1,3-Benzodioxole-5-methanol
495-76-1 | DTXSID3060089

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.93e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.80e-01

Confidence level: 3.08e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Naphthylamine</div> <div>Measured: 2.46e-04</div> <div>Predicted: 8.75e-04</div>	<div>Image not found</div> <div>Anthracene, 9,10-diphenyl-</div> <div>Measured: 1.86e-06</div> <div>Predicted: 2.38e-10</div>	<div>Image not found</div> <div>Metolcarb</div> <div>Measured: 1.38e-07</div> <div>Predicted: 8.30e-04</div>
<div>Image not found</div> <div>MGK-264</div> <div>Measured: 9.68e-06</div> <div>Predicted: 1.19e-05</div>	<div>Image not found</div> <div>Quinoline</div> <div>Measured: 3.52e-03</div> <div>Predicted: 2.64e-02</div>	